Benzene, 1,1'-(1,3-butadiyne-1,4-diyl)bis-

Other names:	Butadiyne, diphenyl-
	Diphenyl-1,3-butadiyne
	Diphenylbutadiyne
	Diphenyldiacetylene
	1,4-Diphenyl-1,3-butadiyne
	1,4-Diphenylbutadiyne
	1,4-Diphenylbut-1,3-diyne
	Diphenylbiacetylene
	NSC 529170
	1,1'-(1,3-butadiyne-1,4-diyl)bisbenzene
Inchi:	InChI=1S/C16H10/c1-3-9-15(10-4-1)13-7-8-14-16-11-5-2-6-12-16/h1-6,9-12H
InchiKey:	HMQFJYLWNWIYKQ-UHFFFAOYSA-N
Formula:	C16H10
SMILES:	C(C#Cc1ccccc1)#Cc1ccccc1
Mol. weight [g/mol]:	202.25
CAS:	886-66-8

Physical Properties

Property code	Value	Unit	Source
chs	-8266.20 ± 1.70	kJ/mol	NIST Webbook
chs	-8243.00 ± 1.00	kJ/mol	NIST Webbook
gf	714.26	kJ/mol	Joback Method
hf	644.09	kJ/mol	Joback Method
hfus	31.52	kJ/mol	Joback Method
hvap	60.07	kJ/mol	Joback Method
ie	7.80	eV	NIST Webbook
ie	8.23	eV	NIST Webbook
ie	7.90 ± 0.08	eV	NIST Webbook
log10ws	-4.52		Crippen Method
logp	3.090		Crippen Method
mcvol	171.580	ml/mol	McGowan Method
pc	3184.73	kPa	Joback Method
tb	636.84	K	Joback Method
tc	930.53	K	Joback Method
tf	359.90 ± 2.00	K	NIST Webbook
vc	0.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	389.45	J/mol×K	636.84	Joback Method
cpg	406.82	J/mol×K	685.79	Joback Method
cpg	422.57	J/mol×K	734.74	Joback Method
cpg	436.84	J/mol×K	783.69	Joback Method
cpg	449.75	J/mol×K	832.63	Joback Method
cpg	461.44	J/mol×K	881.58	Joback Method
cpg	472.05	J/mol×K	930.53	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C886668&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume